Theory for derivation of the expressions for Douglas-Gunn Alternating Direction Implicit (DG-ADI) method for solving the inhomogeneous heat diffusion equation on a rectangular cuboid finite element grid

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March 9, 2019

1 Heat equation

t is the time. The remaining quantities are considered functions of space: The volumetric heat capacity c_{VHC}, with units of $\frac{\mathrm{J}}{\mathrm{m}^3\mathrm{K}}$, the temperature T with units of K, the rate of heat deposition per unit volume per unit time q with units of $\frac{\mathrm{W}}{\mathrm{m}^3\mathrm{s}}$ and the thermal conductivity k, with units of $\frac{\mathrm{W}}{\mathrm{m}\cdot\mathrm{K}}$.

The heat diffusion equation is

$$c_{\mathrm{VHC}}\frac{dT}{dt} = \nabla \cdot (k\nabla T) + q \tag{1}$$

2 Discretization in 1D

Let k_{x+} denote the effective thermal conductivity for heat flow between a voxel and its neighbor in the plus x direction: $k_{x_+} = \frac{2k_ik_{i+1}}{k_i+k_{i+1}}$. Similarly, $k_{x_-} = \frac{2k_{i-1}k_i}{k_{i-1}+k_i}$.

Writing the equation in 1D yields

$$c_{\mathrm{VHC}}\frac{dT}{dt} = \frac{d}{dx}\left(k\frac{d}{dx}T\right) + q \tag{2}$$

Using the notation T^n to denote the temperature at time step n, we can discretize the above as

$$c_{\mathrm{VHC}}\frac{\Delta T}{\Delta t} = \frac{\Delta}{\Delta x}\left(k\frac{\Delta}{2\Delta x}\left(T^n + T^{n+1}\right)\right) + q \tag{3}$$

where we have chosen to use the mean $\frac{1}{2}\left(T^n + T^{n+1}\right)$ as the estimate of the temperature.

We can expand this to get

$$
\begin{aligned}
c_{\mathrm{VHC}}\frac{T^{n+1}-T^{n}}{\Delta t} &= \frac{1}{2\Delta x^2}\Delta\left(k\Delta\left(T^n+T^{n+1}\right)\right)+q \\
= \frac{1}{2\Delta x^2}&\left(k_{x_+}\left(T^n_{i+1}+T^{n+1}_{i+1}-T^n_i-T^{n+1}_i\right)-k_{x_-}\left(T^n_i+T^{n+1}_i-T^n_{i-1}-T^{n+1}_{i-1}\right)\right)+q
\end{aligned} \tag{4}
$$

Moving the terms with time step $n+1$ to the left hand side:

$$
\begin{aligned}
&-\frac{k_{x_+}}{2\Delta x^2}T^{n+1}_{i+1}+\left(\frac{c_{\mathrm{VHC}}}{\Delta t}+\frac{k_{x_+}+k_{x_-}}{2\Delta x^2}\right)T^{n+1}_i-\frac{k_{x_-}}{2\Delta x^2}T^{n+1}_{i-1} \\
&=\frac{k_{x_+}}{2\Delta x^2}T^{n}_{i+1}+\left(\frac{c_{\mathrm{VHC}}}{\Delta t}-\frac{k_{x_+}+k_{x_-}}{2\Delta x^2}\right)T^{n}_i+\frac{k_{x_-}}{2\Delta x^2}T^{n}_{i-1}+q
\end{aligned} \tag{5}
$$

Representing the temperatures and the heat deposition rate as column vectors, we can write the equation in terms of tridiagonal matrix multiplication and column vector addition

$$
M_{\mathrm{LHS}}T^{n+1}=M_{\mathrm{RHS}}T^n+q \tag{6}
$$

where the matrices for insulating boundaries are (example shown for a 5-element grid)

$$
M_{\mathrm{LHS}}=\begin{bmatrix}
\frac{c_{\mathrm{VHC}}}{\Delta t}+\frac{k_{x_+}}{2\Delta x^2} & -\frac{k_{x_+}}{2\Delta x^2} & 0 & 0 & 0 \\
-\frac{k_{x_-}}{2\Delta x^2} & \frac{c_{\mathrm{VHC}}}{\Delta t}+\frac{k_{x_+}+k_{x_-}}{2\Delta x^2} & -\frac{k_{x_+}}{2\Delta x^2} & 0 & 0 \\
0 & -\frac{k_{x_-}}{2\Delta x^2} & \frac{c_{\mathrm{VHC}}}{\Delta t}+\frac{k_{x_+}+k_{x_-}}{2\Delta x^2} & -\frac{k_{x_+}}{2\Delta x^2} & 0 \\
0 & 0 & -\frac{k_{x_-}}{2\Delta x^2} & \frac{c_{\mathrm{VHC}}}{\Delta t}+\frac{k_{x_+}+k_{x_-}}{2\Delta x^2} & -\frac{k_{x_+}}{2\Delta x^2} \\
0 & 0 & 0 & -\frac{k_{x_-}}{2\Delta x^2} & \frac{c_{\mathrm{VHC}}}{\Delta t}+\frac{k_{x_-}}{2\Delta x^2}
\end{bmatrix} \tag{7}
$$

$$
M_{\mathrm{RHS}}=\begin{bmatrix}
\frac{c_{\mathrm{VHC}}}{\Delta t}-\frac{k_{x_+}}{2\Delta x^2} & \frac{k_{x_+}}{2\Delta x^2} & 0 & 0 & 0 \\
\frac{k_{x_-}}{2\Delta x^2} & \frac{c_{\mathrm{VHC}}}{\Delta t}-\frac{k_{x_+}+k_{x_-}}{2\Delta x^2} & \frac{k_{x_+}}{2\Delta x^2} & 0 & 0 \\
0 & \frac{k_{x_-}}{2\Delta x^2} & \frac{c_{\mathrm{VHC}}}{\Delta t}-\frac{k_{x_+}+k_{x_-}}{2\Delta x^2} & \frac{k_{x_+}}{2\Delta x^2} & 0 \\
0 & 0 & \frac{k_{x_-}}{2\Delta x^2} & \frac{c_{\mathrm{VHC}}}{\Delta t}-\frac{k_{x_+}+k_{x_-}}{2\Delta x^2} & \frac{k_{x_+}}{2\Delta x^2} \\
0 & 0 & 0 & \frac{k_{x_-}}{2\Delta x^2} & \frac{c_{\mathrm{VHC}}}{\Delta t}-\frac{k_{x_-}}{2\Delta x^2}
\end{bmatrix} \tag{8}
$$

in which c_{VHC}, k_{x_+}, and k_{x_-} in the i'th row in both matrices are to be evaluated at the spatial position of the i'th pixel/voxel.

The matrices for heat sinked boundaries are

$$M_{\text{LHS}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -\frac{k_{x_-}}{2\Delta x^2} & \frac{c_{\text{VHC}}}{\Delta t} + \frac{k_{x_+}+k_{x_-}}{2\Delta x^2} & -\frac{k_{x_+}}{2\Delta x^2} & 0 & 0 \\ 0 & -\frac{k_{x_-}}{2\Delta x^2} & \frac{c_{\text{VHC}}}{\Delta t} + \frac{k_{x_+}+k_{x_-}}{2\Delta x^2} & -\frac{k_{x_+}}{2\Delta x^2} & 0 \\ 0 & 0 & -\frac{k_{x_-}}{2\Delta x^2} & \frac{c_{\text{VHC}}}{\Delta t} + \frac{k_{x_+}+k_{x_-}}{2\Delta x^2} & -\frac{k_{x_+}}{2\Delta x^2} \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{9}$$

$$M_{\text{RHS}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ \frac{k_{x_-}}{2\Delta x^2} & \frac{c_{\text{VHC}}}{\Delta t} - \frac{k_{x_+}+k_{x_-}}{2\Delta x^2} & \frac{k_{x_+}}{2\Delta x^2} & 0 & 0 \\ 0 & \frac{k_{x_-}}{2\Delta x^2} & \frac{c_{\text{VHC}}}{\Delta t} - \frac{k_{x_+}+k_{x_-}}{2\Delta x^2} & \frac{k_{x_+}}{2\Delta x^2} & 0 \\ 0 & 0 & \frac{k_{x_-}}{2\Delta x^2} & \frac{c_{\text{VHC}}}{\Delta t} - \frac{k_{x_+}+k_{x_-}}{2\Delta x^2} & \frac{k_{x_+}}{2\Delta x^2} \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{10}$$

where furthermore the edge values of q must be zero.

To calculate the temperature T^{n+1}, one can calculate first the right hand side of Eq. 6 by simple matrix multiplication and addition and then solve the remaining system of linear equations for T^{n+1} using, for example, the "matrix left division" of MATLAB.

3 Discretization in 2D